WP 1 – Strategic Development of the CAPITA ERANET, its Programme and its Consortium

Deliverable 1.3 – Applied Catalysis and Process Technology Roadmap 2010 – 2015

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1. Introduction

In order to address outstanding challenges in catalytic and process technological research via the activities within the ERA-NET CAPITA and beyond, the European and global progress in RTD have been analysed, and interim and long-term visions developed. The roadmap should serve as a guide, indicating the requirements in applied catalysis and process technology which are vital for addressing societal and industrial needs in energy, in environmental concerns for transportation and the quality of life and in sustainable chemistry for clean processes for fine chemicals and industrial intermediates and the switch from petrochemical feeds to recycled or renewable feeds.

Several methods exist for developing roadmaps and they differ a lot concerning the numbers of involved persons and the working hours needed. Nevertheless, the general procedure remains the same. The key questions reflect the actual situation and the future aspirations, identify the barriers to progress and finally lead to the solutions and the way forward. The CAPITA's Advisory Group on Innovation and Technology was involved in the roadmapping activities that were especially discussed during two workshops (Paris May 2013 and Brussels February 2014). The following descriptions are also based on documents provided by scientific organisations or activities and by key persons of funding organisations and researchers.

2. The CAPITA's Roadmap: general context and content

Catalytic processes were the key enabling technology of the 20th century and continue to be in the dawn of the 21th century. Thanks to the application of catalysis, human society has had access to fertilisers, fuels, feedstocks, pharmaceuticals, plastics and polymers, agrichemicals, dyestuffs, in fact just about everything produced by the industries using chemistry, or used in their operations. Applied catalysis is also central to control of pollution, most notably in treating exhaust gases from petrol powered road vehicles.

The economic impact of catalysis is quite staggering. The market for catalysts is estimated at about 15 billion Euro per annum, but the value of the goods and services offered by catalysis are >1000 times greater, approaching 20 trillion Euro or 40% of global GDP.

The case for the importance of catalysis continuing into the 21st century is also compelling. Putting industrial society onto a more sustainable footing will require a range of new clean catalytic platform technologies for the production of liquid fuels, chemicals and pharmaceuticals, and materials, using recycled or renewable raw materials and closed cycle, low hazard manufacturing systems. Catalysis is one of the most important technologies for new process design and research. Catalysis is also fundamental to the design and operation of fuel cells, to certain energy storage systems, and to emergent ideas like distributing the manufacture of chemicals to the point of use. It is evident that the organisations that create and exploit the new catalytic platform technologies will not only make a major contribution to sustainable development, but will also create a brand new business.

That new catalytic processes have the potential to become disruptive new platform technologies is not just because of the change in feedstock and market situation. New approaches to process technology, especially process intensification using structured reactors and microreactors, are part of a paradigm shift in chemical processing, where the plant can be optimised around the chemistry, rather than making the chemistry fit within the scope of plant availability. The potential of catalysis to control the rate and direction of a chemical reaction down to the finest levels of the purity and structure of a product (even its stereochemistry) fits precisely with this approach. Similarly, many of the developments in nanotechnology are starting to bring a precision to the design of catalysts themselves, which will optimise the precision and control within a chemical process far beyond the levels currently reached in most catalytic technologies, and will also open routes to new process possibilities. The 21st century's need for new chemical manufacturing technology will be satisfied by a revolution in process technology.

The CAPITA roadmap starts below with a brief recall of the outcome of the ACENET's project (previous ERA-NET on catalysis carried out within FP6, the 6th European Framework Programme), the results of the first CAPITA call within FP7, followed by an assessment of catalysis-connected activities and calls developed within the 7th European Framework programme (section 3). The visions outlined in the new Horizon 2020 European programme (H2020) and in several catalytic and chemical strategy papers are next summarised (section 4). Then, the main expected contributions of catalysis to overcome Europe's societal challenges are collected (section 5), also reflecting the national priorities identified by the CAPITA's consortium members and the participants in the CAPITA's Meetings on "European catalysis strategy and cooperation and International collaboration" (16 May 2013 in Paris, newsletter August 2013, Appendix 1) and "Topics in European Catalysis" (28 February 2014 in Brussels, newsletter March 2014, Appendix 2).

3. Recent activities in catalysis and process technology

3.1 The ACENET projects

The previous ERA-NET on applied catalysis, ACENET (**A**pplied **C**atalysis for **E**urope **NET**work), started in 2004 within FP6 and it continued until 2010. A call for project proposals was launched in 2007, with the ambition to generate transnational research projects on catalysis having an applied character and clear industrial interest. The call was entitled: "Innovative, sustainable catalytic processes with improved energy and carbon efficiency". A project monitoring system was established.

The granted projects covered a large variety of catalysis-related disciplines and offered great potential for innovation and industrial exploitation. A total of 3.7 Million € was allocated, and six projects starting end 2008 or early 2009 were funded (see list below), with partners from seven countries (France, Germany, Greece, Netherlands, Poland, Portugal and Spain). 100% proofs of concepts were achieved and 5 to 26 publications and 0 to 2 patents were produced per project.

Table 1: The ACENET projects

Title and Acronym	**Participating Countries**	**Project coordinator**
Alkanes to light olefins via novel catalysts and process schemes (AL2OL)	DE, GR, ES	Prof. Johannes A. Lercher, TUM, Munich, Germany
Heterogeneous catalysis for the conversion of solid biomass into renewable fuels and chemicals (HECABIO)	GR, ES, FR, NL	Dr Angelos A Lappas, CPERI/CERTH, Thessaloniki, Greece
Methane activation as a route to CO_2 remediation: the integration of dry reforming into Fischer-Tropsch fuel production plants (METACOOR)	FR, DE, ES	Dr Christophe Copéret, ESCPE/CNRS, Lyon, France
Hydrogen from bio-alcohols: An efficient route for hydrogen production via novel reforming catalysts (NUCAT4HYDROGEN)	GR, PL, ES	Dr Theophilos Ioannides, ICE-HT/FORTH, Patras, Greece
Simultaneous production of hydrogen and C2 hydrocarbons in solid oxide membrane reactors (SIPROHYM)	GR, NL, ES, PT	Prof. Michael Stoukides, CPERI /CERTH, Thessaloniki, Greece
Catalysis by regenerable super bases (SUBACA)	FR, NL, ES	Dr Francois Figueras, IRCELYON, Lyon, France

3.2 The CAPITA projects

The ERA-NET CAPITA started in 2012 within FP7 and it continued until 2014. A call for project proposals was launched in 2013, with the ambition to generate transnational research projects on catalysis having an applied character and clear industrial interest. The call was entitled: “Innovative catalysis for the monetization of low value carbon”.

The granted projects covered a large variety of catalysis-related disciplines and offered great potential for innovation and industrial exploitation. A total of 2.2 Million € of the call budget and another 120 Thousand € of private funding was allocated, and three projects starting end 2013 or early 2014 were funded (see list below), with partners from six countries (Flanders, Greece, Italy, Netherlands and Spain).

Table 2: The CAPITA projects

Title and Acronym	**Participating Countries**	**Project coordinator**
Valorization of CARbon DIOxide containing industrial streams via non-conventional catalytic systems and SOLarized processes (CARDIOSOL)	GR, IT	Dr George Skevis, APTL/CERTH, Thessaloniki, Greece
CO2 and H2O toward methanol synthesis at atmospheric pressure in co-ionic electrochemical membrane reactors (GREEN MEOH)	ES, GR, NL	Assoc. Prof. F. Dorado Fernández, UCLM, Castilla-La-Mancha, Spain
WAste bio-feedstocks hydro-Valorisation processes (WAVES)	GR, ES, NL, BE, IT	Dr A. Lappas, CPERI/CERTH, Thessaloniki, Greece

3.3 Catalysis and Process Technology topics in FP7, NMP

An important strategic objective of the 7th Framework Programmes for Research (FP7, 2007-2013) was to strengthen the scientific and technological bases of European industry and to encourage its international competitiveness. In the specific programme “Cooperation”, especially in the theme 4 “Nanosciences, Nanotechnologies, Materials and Production technologies” (**NMP**), catalysis and process technology topics were continuously included in the work programmes. Throughout the duration of FP7, 15 topics were launched in NMP in this area, leading to 40 projects with more than 500 partners from 33 countries, gaining about 220 million € EC funding (on a total of 3.5 billion initially planned for NMP, i.e. more than 6% of the effort).

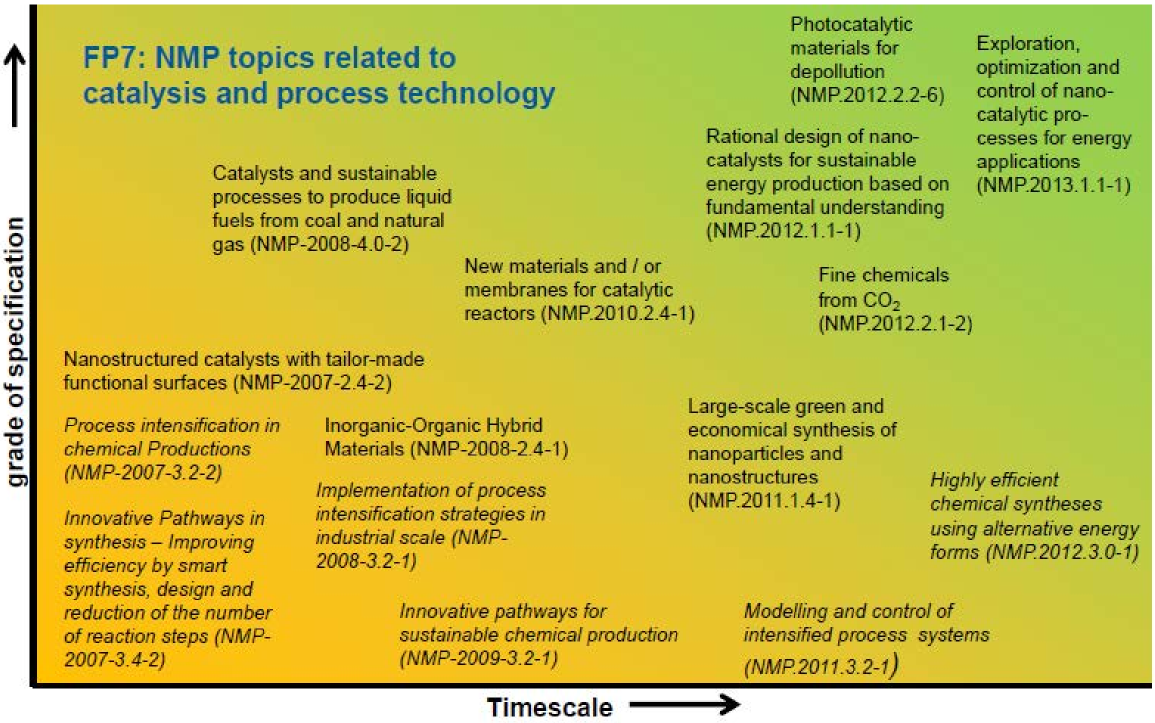

Figure 1: NMP topics related to catalysis and process technology, released within FP7

As shown in **Figure 1**, a tendency from general to more specified objectives can be drawn during the lifespan of FP7 on these topics. This is not really surprising and can be understood as a smooth transition towards Horizon 2020, the EU's new research and innovation programme. The topics in process technology, written in italic letters, followed a multi-annual plan and are highly linked together. **Table 3** provides details on the 40 funded projects with topics in catalysis and process technology, listed according to the published call they refer to. Specific website addresses are also indicated for most of these projects, as well as the CORDIS website of the EC for funded FP7 projects, in which periodic and final FP7 reports can be found for each project.

Table 3: Projects in catalysis and process technology funded under FP7 in NMP

Call topic	*Acronym* and Title	*# partners* duration	Coordinator / Adm. Contact	Website(s)
NMP-2007-2.4-2 Nanostructured catalysts with tailor-made functional surfaces	***ERUDESP*** Development of electrochemical reactors using dehydrogenases for enantiopure synthon preparations	*6 partners* 2008-07-01 / 2011-06-30	Prof. Dr. Rolf HEMPELMANN, Physical Chemistry, Saarland University,Saarbruecken, Germany	www.erudesp.eu/ http://cordis.europa.eu/project/rcn/87775_en.html
	HiCat Hierarchically organized metal organic catalysts for continuous and multi-batch processes	*8 partners* 2008-09-01 / 2011-08-31	Dr. Juergen CZWALINNA, Evonik Industries AG, Essen, Germany	http://cordis.europa.eu/project/rcn/88894_en.html
NMP-2007-3.2-2 Process intensification in chemical Productions	***CAEC*** Continuous Annular Electro-Chromatography	*8 partners* 2008-09-01 / 2012-08-31	Prof. Andrzej GÓRAK, Technische Universität Dortmund, Dpt. Biochemical and Chemical Engineering, Dortmund, Germany	http://caec.bci.tu-dortmund.de/ http://cordis.europa.eu/project/rcn/88731_en.html
	PILLS Process intensification methodologies for liquid-liquid systems in structured equipment	*10 partners* 2009-01-01 / 2012-03-31	Drs. Steve FLETCHER / Rebecca FARNELL, Chemistry innovation limited, Burlington House Picadilly, London, United Kingdom	www.fp7pills.eu/ http://cordis.europa.eu/project/rcn/89659_en.html
	ROC Radiochemistry on chip	*5 partners* 2008-09-01 /	Ms. Paola COREZZOLA, Consiglio Nazionale della	http://cordis.europa.eu/project/rcn/86709_en.html

		2011-08-31	Ricerche , Roma, Italy	
NMP-2007-3.4-2 Innovative Pathways in synthesis – Improving efficiency by smart synthesis, design and reduction of the number of reaction steps	***EFFECTS*** Efficient environmental-friendly electro-ceramics coating technology and synthesis	*8 partners* 2008-10-01 / 2011-09-30	Prof. dr. I. Van DRIESSCHE, Universiteit Gent - Ghent University, Dep. Inorganic, Gent, Belgium	http://cordis.europa.eu/project/rcn/89597_en.html
	EUMET Olefin metathesis as a practical synthetic tool	*10 partners* 2008-11-01 / 2012-10-31	Prof. Steven P. NOLAN, University of St Andrews, St Andrews Fife, Scotland, United Kingdom	www.eumet.unisa.it/ http://cordis.europa.eu/project/rcn/90238_en.html
	INTENANT Integrated synthesis and purification of single enantiomers	*11 partners* 2008-06-01 / 2011-05-31	Prof. Andreas SEIDEL-MORGENSTERN, Max Plank Gesellschaft zur Förderung der Wissenschaften e.V., Munich, Germany	http://cordis.europa.eu/result/rcn/45395_en.html
NMP-2008-2.4-1 Inorganic-Organic Hybrid Materials	***MACADEMIA*** MOFs as catalysts and adsorbents: discovery and engineering of materials for industrial applications	*17 partners* 2009-07-01 / 2013-06-30	Dr. Francis LUCK, Total S.A., Courrbevoie, France	www.macademia-project.eu/ http://cordis.europa.eu/project/rcn/92878_en.html
	NanoMOF Nanoporous Metal-Organic Frameworks for production	*17 partners* 2009-06-01 / 2013-05-31	Dr. Wulf GRÄHLERT, Fraunhofer-Institut für Werkstoff- und Strahltechnik IWS, Dresden, Germany	www.nanomof-project.eu/ http://cordis.europa.eu/result/rcn/90519_fr.html
	ORION Orderd inorganic-organic hybrids using ionic liquids for emerging applications	*17 partners* 2009-10-01 / 2013-09-30	Mr. Jon LACUNZA, Fundacion Cidetec, Donostia – San Sebastian, Spain	www.cidetec.es/ORION/index.html http://cordis.europa.eu/project/rcn/107704_en.html
NMP-2008-3.2-1 Implementation of process intensification strategies in industrial scale	***COPIRIDE*** Combining process intensification-driven manufacture of microstructured reactors and process design regarding to industrial dimensions and environment	*16 partners* 2009-09-01 / 2013-08-31	Dr. Patrick LÖB, Institut für Mikrotechnik Mainz GmbH, Mainz, Germany	www.copiride.eu/ http://cordis.europa.eu/project/rcn/92652_en.html
	F³ Factory Flexible, fast and future production processes	*25 partners* 2009-06-01 / 2013-05-31	Dr. Sigurd BUCHHOLZ, Bayer Technology Services GmbH, Leverkusen, Germany	www.f3factory.com http://cordis.europa.eu/project/rcn/92587_en.html
NMP-2008-4.0-2 Catalysts and sustainable processes to produce liquid fuels from coal and natural gas	***NEXT-GTL*** Innovative catalytic technologies & materials for next gas to liquid processes	*23 partners* 2009-11-01 / 2013-10-31	Prof. Gabriele CENTI, Consorzio interuniversitario nazionale per las scienza e tecnologia dei materiali, Firenze, Italy	http://cordis.europa.eu/project/rcn/93080_en.html
	OCMOL Oxidative coupling of Methane followed by Oligomerization to Liquids	*17 partners* 2009-09-01 / 2014-08-31	Prof. Guy B. MARIN, Ghent University, Gent, Belgium	www.ocmol.eu http://cordis.europa.eu/project/rcn/92879_en.html
NMP-2009-3.2-1 Innovative pathways for sustainable chemical production	***INCAS*** Integration of Nanoreactor and multisite CAtalysis for a Sustainable chemical production	*11 partners* 2010-10-01 / 2014-09-30	Dr. Claudia BETTACCINI, Consorzio interuniversitario nazionale per las scienza e tecnologia dei materiali, Firenze, Italy	www.incasproject.eu/ http://cordis.europa.eu/project/rcn/96186_en.html
	POLYCAT Modern polymer-based catalysts and microflow conditions as key elements of innovations in fine chemical syntheses	*19 partners* 2010-10-01 / 2014-03-31	Dr. Patrick LÖB, Institut für Mikrotechnik Mainz GmbH, Mainz, Germany	www.polycat-fp7.eu http://cordis.europa.eu/project/rcn/96187_en.html
	SYNFLOW Innovative	*19 partners*	Prof. Ernst SCHMACHTENBERG Rheinisch-Westfählische	www.synflow.eu/

	Synthesis in Continuous-Flow Processes for Sustainable Chemical Production	2010-09-01 / 2014-08-31	Technische Hochschule Aachen (RWTH), Aachen, Germany	http://cordis.europa.eu/project/rcn/96217_en.html
NMP.2010.2.4-1 New materials and / or membranes for catalytic reactors	***CARENA*** Catalytic membrane Reactors based on New mAterials for C1-C4 valorization	*18 partners* 2011-06-01 / 2015-05-31	Mr. Arend DE GROOT, Stichting energieonderzoek centrum Nederland, Petten, The Netherlands	www.carenafp7.eu/ http://cordis.europa.eu/project/rcn/99119_en.html
	DEMCAMER Design and Manufacturing of Catalytic Membrane Reactors by developing new nano-architectured catalytic and selective membrane materials	*18 partners* 2011-07-01 / 2015-06-30	Dr. José-Luis VIVIENTE, Tecnalia, Materials for Energy Department, Donostia – San Sebastián, Spain	www.demcamer.org/ http://cordis.europa.eu/project/rcn/99344_en.html
NMP.2011.1.4-1 Large-scale green and economical synthesis of nanoparticles and nanostructures	***BUONAPART-E*** Better Upscaling and Optimization of Nanoparticle and Nanostructure Production by Means of Electrical Discharges	*21 partners* 2012-02-01 / 2016-01-31	Ms. Sandra KRAMM (Ms.), Universität Duisburg-Essen, Essen, Germany	www.buonapart-e.eu/ http://cordis.europa.eu/project/rcn/102134_en.html
	SHYMAN Sustainable Hydrothermal Manufacturing of Nanomaterials	*18 partners* 2012-05-01 / 2016-04-30	Mr. Paul CARTLEDGE, The University of Nottingham, Nottingham, United Kingdom	www.shyman.eu/ http://cordis.europa.eu/project/rcn/103330_en.html
NMP.2011.3.2-1 Modelling and control of intensified process systems	***COOPOL*** Control and Real-Time Optimisation of Intensive Polymerisation Processes	*7 partners* 2012-03-01 / 2015-02-28	Prof. David HADDLETON, Department of Chemistry, University of Warwick, Coventry, United Kingdom	www.coopol.eu/ http://cordis.europa.eu/project/rcn/102445_en.html
	OPTICO Model-based optimization & Control for process-intensification in chemical and biopharmaceutical systems	*13 partners* 2012-02-01 / 2015-01-31	Prof. Costas KIPARISSIDES, Centre for Research and technology Hellas (CERTH), Thermi-Thessaloniki, Greece	http://opticoproject.eu/2219EA10.en.aspx http://cordis.europa.eu/project/rcn/102169_en.html
NMP.2012.1.1-1 Rational design of nano-catalysts for sustainable energy production based on fundamental understanding	***chipCAT*** Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology	*8 partners* 2012-12-01 / 2016-11-30	Prof. Vladimir MATOLIN (Professor), Univerzita Karlova v Praze, Prague, Czech Republic	http://chipcat.eu/ http://cordis.europa.eu/project/rcn/106161_en.html
	DECORE Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of catalyst / support assembly for high temperature operation	*7 partners* 2013-01-01 to 2016-12-31	Ms. Anna MODENATO, Universita degli Studi di Padova, Padova, Italy	http://cordis.europa.eu/project/rcn/106197_en.html
	SOLAROGENIX Visible-Light Active Metal Oxide Nano-catalysts for Sustainable Solar Hydrogen Production	*9 partners* 2013-01-01 / 2015-12-31	Dr. Christian KLAR (Dr), Universität zu Köln, Cologne, Germany	www.solarogenix.eu/ http://cordis.europa.eu/project/rcn/106812_en.html
	SusFuelCat Sustainable fuel production by aqueous phase reforming understanding catalysis and hydrothermal stability of carbon supported noble metals	*10 partners* 2013-01-01 / 2016-12-31	Ms. Franziska MÜLLER, Friedrich-Alexander Universität Erlagen Nürnberg, Erlangen, Germany	www.susfuelcat.eu/ http://cordis.europa.eu/project/rcn/106702_en.html
NMP.2012.2.1-2 Fine chemicals from CO2	***CEOPS*** CO2 - Loop for Energy storage and conversion to Organic chemistry Processes through advanced catalytic Systems	*10 partners* 2013-02-01 / 2016-01-31	Dr. Stephanie THOLLON, Commissariat a l'atomique et aux enrgies alternatives (CEA), Paris, France	www.ceops-project.eu/ http://cordis.europa.eu/project/rcn/105903_en.html

	CyclicCO2R Production of Cyclic Carbonates from CO2 using Renewable Feedstocks	*8 partners* 2013-01-01 / 2016-12-31	Dr. Erin KIMBALL, Nederlandse Organisatie voor toegepast natuurwetenschappelijk onderzoek – TNO, Delft, The Netherlands	www.cyclicco2r.eu/ http://cordis.europa.eu/project/rcn/106539_en.html
	Eco2CO2 Eco-friendly biorefinery fine chemicals from CO2 photo-catalytic reduction	*9 partners* 2012-12-01 / 2016-05-31	Prof. Guido SARACCO, Politecnico di Torino, Torino, Italy	http://eco2co2.org/default.aspx http://cordis.europa.eu/project/rcn/105900_en.html
NMP.2012.2.2-6 Photocatalytic materials for depollution	***4G-PHOTOCAT*** Fourth generation photo-catalysts: nano-engineered composites for water decontamination in low-cost paintable photoreactors	*11 partners* 2013-01-01 / 2015-12-31	Prof. Radim BERANEK, Ruhr-Universität Bochum (RUB), Bochum, Germany	www.4g-photocat.eu/ http://cordis.europa.eu/project/rcn/105983_en.html
	LIMPID Nanocomposite materials for photocatalytic degradation of pollutants	*12 partners*; 2012-12-01 / 2015-11-30	Dr. Maria Lucia CURRI, Consiglio nazionale delle Ricerche, Roma, Italy	www.limpid-fp7.eu/ http://cordis.europa.eu/project/rcn/106202_en.html
	PCATDES Photocatalytic Materials for the Destruction of Recalcitrant Organic Industrial Waste	*10 partners* 2013-02-01 / 2017-01-31	Dr Philip R. DAVIES, Cardiff University, Cardiff, United Kingdom	www.pcatdes.eu/ http://cordis.europa.eu/project/rcn/106542_en.html
NMP.2012.3.0-1 Highly efficient chemical syntheses using alternative energy forms	***ALTEREGO*** Alternative Energy Forms for Green Chemistry	*8 partners* 2013-01-01 / 2016-06-30	Prof. Andrzej STANKIEWICZ , Technische Universiteit Delft, Delft, The Netherlands	http://cordis.europa.eu/project/rcn/106201_en.html
	InnoREX Continuous, highly precise, metal-free polymerisation of PLA using alternative energies for reactive extrusion	*12 partners* 2012-12-01 / 2016-05-31	Björn BERGMANN, Fraunhofer-Institut für Chemische Technologie ICT Pfinztal, Germany	www.innorex.eu/ http://cordis.europa.eu/project/rcn/106198_en.html
	MAPSYN Microwave, Ultrasonic and Plasma assisted Syntheses	*12 partners* 2012-12-01 / 2016-05-31	Dr. Paul FITZPATRICK, C-Tech Innovation limited, Chester, United Kingdom	http://mapsyn.eu./ http://cordis.europa.eu/project/rcn/106321_en.html
NMP.2013.1.1-1 Exploration, optimization and control of nano-catalytic processes for energy applications	***BIOGO*** Catalytic Partial Oxidation of Bio Gas and Reforming of Pyrolysis Oil (Bio Oil) for an Autothermal Synthesis Gas Production and Conversion into Fuels	*17 partners* 2013-12-01 / 2017-10-31	Prof. Dr. Gunther Kolb Fraunhofer ICT-IMM, Mainz Germany Institut für Mikrotechnik, Mainz, Germany	www.biogo.eu/ http://cordis.europa.eu/project/rcn/110962_en.html
	CASCATBEL CAScade deoxygenation process using tailored nanoCATalysts for the production of BiofuELs from lignocellullosic biomass	*17 partners* 2013-11-01 / 2017-11-01	Dr. David P. Serrano, Fundacion IMDEA Energia, Spain	www.cascatbel.eu/ http://cordis.europa.eu/project/rcn/110687_en.html
	FASTCARD FAST industrialisation by CAtalysts Research and Development	*14 partners* *2014-01-01 / 2017-12-31*	Ms. Tove Lillian Hønstad, Stiftelsen SINTEF Norway	http://cordis.europa.eu/project/rcn/110686_en.html

4. European Vision

4.1 EU 2020 Targets and SPIRE initiative

CAPITA is an ERA-NET within the 7th Framework programme and is therefore acting in the European context. A clear European vision for the next years was recently set by the "**Europe 2020 strategy – a vision of a smart, sustainable and inclusive growth"**,[2] a document where the EU 2020 main targets proposed by the Commission are detailed. These targets are summarised in ***box 1***. This strategy paper outlines that Europe faces a moment of transformation: recovering from the crisis, Europe must now take charge of its future in acting collectively as a Union. That is why transnational collaboration is so important. The ERA-NET activities are a contribution to join forces.

Seven flagship initiatives have been proposed by the Commission to accelerate progress and to deliver the Europe 2020 goals. Catalysis as a key enabling technology can mainly contribute to three of them:

"Innovation Union",[3] to improve framework conditions and access to finance for research and innovation so as to ensure that innovative ideas can be turned into products and services that create growth and jobs.

"Resource efficient Europe",[4] to help decouple economic growth from the use of resources, support the shift towards a low carbon economy, increase the use of renewable energy sources, modernise our transport sector and promote energy efficiency.

"An industrial policy for the globalisation era",[5] with the aim to improve the business environment, notably for SMEs, and to support the development of a strong and sustainable industrial base able to compete globally.

The EU 2020 targets, proposed by the Commission:

– 75 % of the population aged 20-64 should be employed.

– 3% of the EU's GDP should be invested in R&D.

– The "20/20/20" climate/energy targets should be met (including an increase to 30% of emissions reduction if the conditions are right).

– The share of early school leavers should be under 10% and at least 40% of the younger generation should have a tertiary degree.

– 20 million less people should be at risk of poverty.

box 1

In order to achieve the goals set in the flagship initiative "A resource efficient Europe" and in its related "Roadmap to a Resource Efficient Europe" (COM(2011) 571, see below), applied catalysis and new catalytic technologies as well as process technologies will be very important. There is a need for technological improvements to trigger significant transition in energy, industrial, agricultural and transport systems, to ensure the access to water, food and raw materials and to step forward in a "circular economy".

This was also felt by the scientific and industrial community, leading to the **SPIRE initiative**[6] that recently delivered a roadmap for a "**S**USTAINABLE **P**ROCESS **I**NDUSTRY THROUGH **R**ESOURCE AND **E**NERGY EFFICIENCY".[7] This contractual Public-Private Partnership (PPP) initiated in the frame of SusChem, the European Technology Platform for Sustainable Chemistry, is the first-ever cross-sectorial partnership launched between the European Commission and eight industrial sectors, as part of the Horizon 2020 framework programme. Dedicated to innovation in resource and energy efficiency, its target is to drastically reduce the environmental footprint and to increase competitiveness of industry by "doing more and/or better with less". Therefore all stages along the full value chain will be addressed by implementing four key components in feed, process, applications and waste

2 http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=COM:2010:2020:FIN:EN:PDF
3 http://ec.europa.eu/research/innovation-union/
4 http://ec.europa.eu/resource-efficient-europe/
5 http://ec.europa.eu/enterprise/policies/industrial-competitiveness/industrial-policy/
6 http://www.spire2030.eu/
7 http://www.spire2030.eu/uploads/Modules/Publications/spire-roadmap_december_2013_pbp.pdf

box 2

resource, as well as two additional key components with horizontal and outreach activities. The two ambitions of SPIRE for 2030 are summarized in ***box 2***.

SPIRE's two ambition for 2030

1. Reducing fossil energy intensity of up to 30% from current levels;

2. Reducing non-renewable, primary raw material intensity of up to 20% from current levels.

Both ambitions will contribute to efficiency improvement in CO_2 – equivalent footprints of up to 40% by 2030. Potential improvements extend beyond "industry" to all indirectly supplied and dependent economic sectors such as transport, construction, water, electronics etc.

4.2 Relevant EC Strategy Papers and Roadmaps

Further strategy papers and roadmaps are developed by the Commission to tackle the Grand challenges, started with the Lund declaration and triggered by the EU 2020 strategy. Some important documents with regard to catalysis and process technologies are the following:

- ✓ **Energy Roadmap 2050.**[8]
  On 15 December 2011, the European Commission adopted the Communication "Energy Roadmap 2050". The EU is committed to reducing greenhouse gas emissions to 80-95% below 1990 levels by 2050 in the context of necessary reductions by developed countries as a group. In the Energy Roadmap 2050, the Commission explores the challenges posed by delivering the EU's decarbonisation objective while at the same time ensuring security of energy supply and competitiveness. The Energy Roadmap 2050 is the basis for developing a long-term European framework together with all stakeholders.

- ✓ **Low-carbon economy: SET-Plan towards a Low Carbon future.**[9]
  The SET-Plan establishes an energy technology policy for Europe. It's a strategic plan to accelerate the development and deployment of cost-effective low carbon technologies. The plan comprises measures relating to planning, implementation, resources and international cooperation in the field of energy technology.

- ✓ **Materials Roadmap Enabling Low-Carbon Energy Technologies.**[10]
  The Materials Roadmap addresses the technology agenda of the SET-Plan by proposing a comprehensive European programme on materials research and innovation enabling low-carbon energy technologies for the next 10 years. Its starting point is the sector's ambitions and technology challenges addressed in the SET-Plan initiatives. The energy technologies considered are: wind, photovoltaic, concentrating solar power, geothermal, electricity storage, electricity grids, bio-energy, novel materials for the fossil fuel energies sector (including carbon capture and storage), hydrogen and fuel cells, nuclear fission and energy efficient materials for buildings.

- ✓ **Roadmap to a Resource Efficient Europe.**[11]
  The Roadmap to a Resource Efficient Europe (COM(2011) 571) outlines how we can transform Europe's economy into a sustainable one by 2050. It proposes ways to increase resource productivity and decouple economic growth from resource use and its environmental impact. It illustrates how policies interrelate and build on each other. Areas where policy action can make a real difference are a particular focus; specific bottlenecks like inconsistencies in policy and market failures are tackled to ensure that policies are all going in the same direction. Cross-cutting themes such as addressing prices that do not

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8 http://ec.europa.eu/energy/publications/doc/2012_energy_roadmap_2050_en.pdf
9 http://ec.europa.eu/energy/publications/doc/2010_setplan_brochure.pdf
10 http://setis.ec.europa.eu/system/files/Materials_Roadmap_EN.pdf
11 http://ec.europa.eu/environment/resource_efficiency/pdf/com2011_571.pdf

reflect the real costs of resource use and the need for more long-term innovative thinking are also in the spotlight. Key resources are analysed from a life-cycle and value-chain perspective. Nutrition, housing and mobility are the sectors responsible for most environmental impacts; actions in these areas are being proposed to complement existing measures. The Resource Efficiency Roadmap provides a framework in which future actions can be designed and implemented coherently. It sets out a vision for the structural and technological change needed up to 2050, with milestones to be reached by 2020. These milestones illustrate what will be needed to put Europe on a path to resource efficient and sustainable growth.

5. National Roadmaps, H2020 context and Recommendations on Actions

5.1 National Roadmaps and integration within H2020

Tapping the full potential of catalysis for innovative technology applications in order to meet the societal challenges has been the underlying stimulus of various recent national or international roadmaps in catalysis, process technologies and/or chemistry. **Table 3** (next page) provides a list of such published roadmaps (ordered according to their publishing date) that were considered in CAPITA's orientations. For the sake of completion, available non-European documents are also reported.

The CAPITA roadmap needs also to be linked to the structures and elements of the EU2020 strategy. In particular, the focus areas must meet the societal challenges identified by Horizon 2020, which list is recalled below:

- Health, demographic change and wellbeing;
- Food security, sustainable agriculture and forestry, marine and maritime and inland water research, and the *Bioeconomy;*
- Secure, *clean and efficient energy;*
- Smart, *green and integrated transport;*
- Climate action, *environment, resource efficiency and raw materials;*
- Europe in a changing world - inclusive, innovative and reflective societies;
- Secure societies - protecting freedom and security of Europe and its citizens.

The *blue marked areas* are those where the CAPITA roadmap is strongly concerned. This is why the presentation below will follow the H2020 societal challenges order, to clarify the strong interconnections between the CAPITA and H2020 priorities. In addition, a horizontal topic concerning development of catalysts and reactor concepts will be added.

5.2 Secure, clean and efficient energy

In a world with a strong – and still increasing - energy demand and where the fossil energy sources are limited, it is necessary to optimize the use of existing fossil resources and to pave the way for renewable resources. The best use of traditional energy resources and the introduction of new abundant and renewable resources require the implementation of new strategies where chemistry and especially catalysis provide the key for solutions.

Of all of the fossil fuels, reserves of crude oil are due to run out first. Therefore, *natural gas* will become more important, not only as fuel but also as raw material for the chemical industry. The development of natural gas will go along with development of the conversion process on the site, which are often off-shore. Hence, this implies the *miniaturisation of the reforming units*. For natural gas from renewable resources such as biogas fermentation, please refer to section 5.3.

Table 4: Recent National and international roadmaps in catalysis

Document Title	Country	Initiated by	Publishing date
Technology Roadmap Catalysis – Catalysis, key to sustainablility[12]	The Netherlands	Ministry of economic Affairs in Netherlands	2001
Basic Research Needs: Catalysis for Energy[13]	The United States	US Department of energy	2007
Australian scientific roadmap for the hydrogen economy[14]	Australia	Australian Academy of Science	2008
Future perspectives in catalysis[15]	The Netherlands	NRSC (Dutch National Research School)	2009
Catalysis – A key technology for sustainable economic growth, 3rd edition[16]	Germany	GECATS (German Catalysis Society)	2010
Overview and Potentials of development of biorefineries[17]	France	ADEME (Agence de l'Environnement et de la Maîtrise de l'Energie)	2010
Biofuels for Transport - Technology Roadmap[18]	International	IEA (International Energy Agency)	2011
Rapport de Conjoncture – Chimie de coordination, interfaces et procédés[19]	France	CNRS (Centre National de la Recherche Scientifique)	2010
Supplement to Roadmap for catalysis research in Germany: Catalysis beyond the roadmap[20]	Germany	GECATS (German Catalysis Society)	2012
Chemistry's Contribution to Energy Efficiency[21]	International	ICCA (International Council of Chemical Associations)	2013
SPIRE Roadmap[22]	Europe	A.SPIRE asbl	2013
Technology Roadmap Energy and GHG Reductions in the Chemical Industry via Catalytic Processes[23]	International	IEA (International Energy Agency) / ICCA (International Council of Chemical Associations) / DECHEMA	2013

12 http://www.eric-aisbl.eu/documents/TRM_Catalysis_Rapport.pdf
13 http://web.anl.gov/catalysis-science/publications/CAT_rpt.pdf
14 www.science.org.au/publications/towards-development-australian-scientific-roadmap-hydrogen-economy
15 http://www.nrsc-catalysis.nl/files/media/scientific_reports/Future_perspectives_in_Catalysis.pdf
16 http://www.gecats.de/gecats_media/Urbanczyk/Katalyse_Roadmap_2010_engl_final.pdf
17 http://www2.ademe.fr/servlet/getDoc?cid=96&m=3&id=80942&p1=02&p2=08&ref=17597
18 http://www.iea.org/publications/freepublications/publication/technology-roadmap-biofuels-for-transport.html
19 http://www.cnrs.fr/comitenational/doc/rapport/2010/14_conj_2010.pdf
20 http://www.dechema.de/dechema_media/Katalyse_Supplement_2012_final-p-4094.pdf
21 http://www.icca-chem.org/ICCADocs/ICCA Roadmap Summary.pdf
22 see section 4.1
23 http://www.iea.org/publications/freepublications/publication/Chemical_Roadmap_2013_Final_WEB.pdf

Hydrogen is one of the most important environmentally safe energy carriers of the future. Catalysis is directly involved in the perspective of *hydrogen as an energy carrier* for its production, purification and conversion in electrochemical fuels. Hydrogen is produced mainly in large industrial units by steam reforming of natural gas (85%) or heavier hydrocarbons. In future, research should focus on the transition to renewable resources such as lignocellulosic biomass (see 5.3)

Concerning hydrogen production and storage, research should contribute to the achievement of fundamental breakthroughs in materials and processes for hydrogen production routes using different primary energy sources. It should also contribute to the understanding of the physical and chemical aspects of processes governing the storage of hydrogen, in particular the interface of hydrogen with materials. Emphasis should be given to catalytic production pathways which contribute to energy security and carbon dioxide mitigation.

The *electrolysis of water vapour* at high temperature for the industrial production of hydrogen used for power fuel cells without emissions of Greenhouse Gases is a promising way, but still optimized processes need to be found, likewise high-pressure electrolysis or gas phase electrolysis. New electrode materials as electrocatalysts with a similary low overvoltage to platinum but cheaper and with good availability would also push the progress in this field.

Although the feasibility of *photocatalytic water splitting* can be demonstrated at the laboratory scale, the way to commercialisation is still challenging. The main hurdle to overcome is the space-time yield, regardless of whether the systems are based on solid catalysts or biochemical/biomimetic concept. New photocatalysts need to be developed / tailored with reduced band gaps (<3 eV) which are sensitive in the range of the visible light and stable under the working conditions.

If hydrogen from renewable sources can be produced, then the next link in the chain of the non-fossil energy of the future is the fuel cell. Research in *fuel cell technology* should contribute in achieving significant, fundamental breakthroughs in the understanding of the physical and chemical aspects of catalyst materials included in the fuel cell stacks. The aim is to reduce fuel cell stack and system cost, and improving performance and durability of existing fuel cell technologies. Research should be dedicated to novel materials, including nano-structured materials and integrated nano-scale architectures for catalysts.

In the Netherlands, the following topics summarized under the heading “Catalysis for storing electrons /photons, solar fuels and resource utilisation” are of high priority:

- Solar fuels/chemicals, catalysis for CO_2 and water.
- Storing electrons chemically (considering the ever-increasing electrification of transport), catalysis for batteries.
- Alternative stimuli for catalysis (photons, electrons).

In Spain, special attention is put on topics concerning hydrogen production:

- Development of active and stable catalysts for the reformation of hydrocarbons in decentralized systems.
- Provision of highly active and selective catalysts for the purification of synthesis gas.
- Decentralized, climate-neutral hydrogen production from cultivated biomass or from the exploitation of secondary materials via autothermic reformation.
- Development of active and stable catalysts for production of pure hydrogen by direct decomposition of biogas (methane).

The German Catalysis Society identified research requirements similar to those of Spain in the field of hydrogen and following additional issues:

- Improvement of water electrolysis processes, both in terms of the electrocatalysts and in term of process control.
- Long-term research projects looking into photocatalytic water splitting with new catalyst systems to create a simple way to supply the hydrogen required for the hydrogen industry.

Additional aspects concerning electrolytic water cleavage are also highlighted in the Technology Roadmap of the IEA. Thus, although nickel is used predominantly as catalytic active phase in this process, platinum would be better in terms of energy efficiency, but would raise the costs. Therefore, to bring significant progress in electrolytic water cleavage, there is a need of cheap electrode materials with a low overvoltage similar to that of platinum. Moreover, new process variants, such as high-pressure electrolysis or gas phase electrolysis should be tested and optimized.

In the status report 2010 of CNRS (France), following options are given concerning energy:

- Miniaturization / intensification of reforming units for the processing of natural gas.
- Management of impurities (Sulfur, organic and inorganic) and their variable composition in natural gas and heavy petroleum fractions in cruide oil for the synthesis of fuel via Fischer-Tropsch.
- Overcome the technological hurdles in the electrolysis of water vapour at high temperature.
- Shifting the photocatalytic water splitting to visible light and discovery of materials with band gap less than 3 eV.
- Other forms of non-thermal activation reaction media such as cold plasmas or voltaic assistance in photocatalysis.

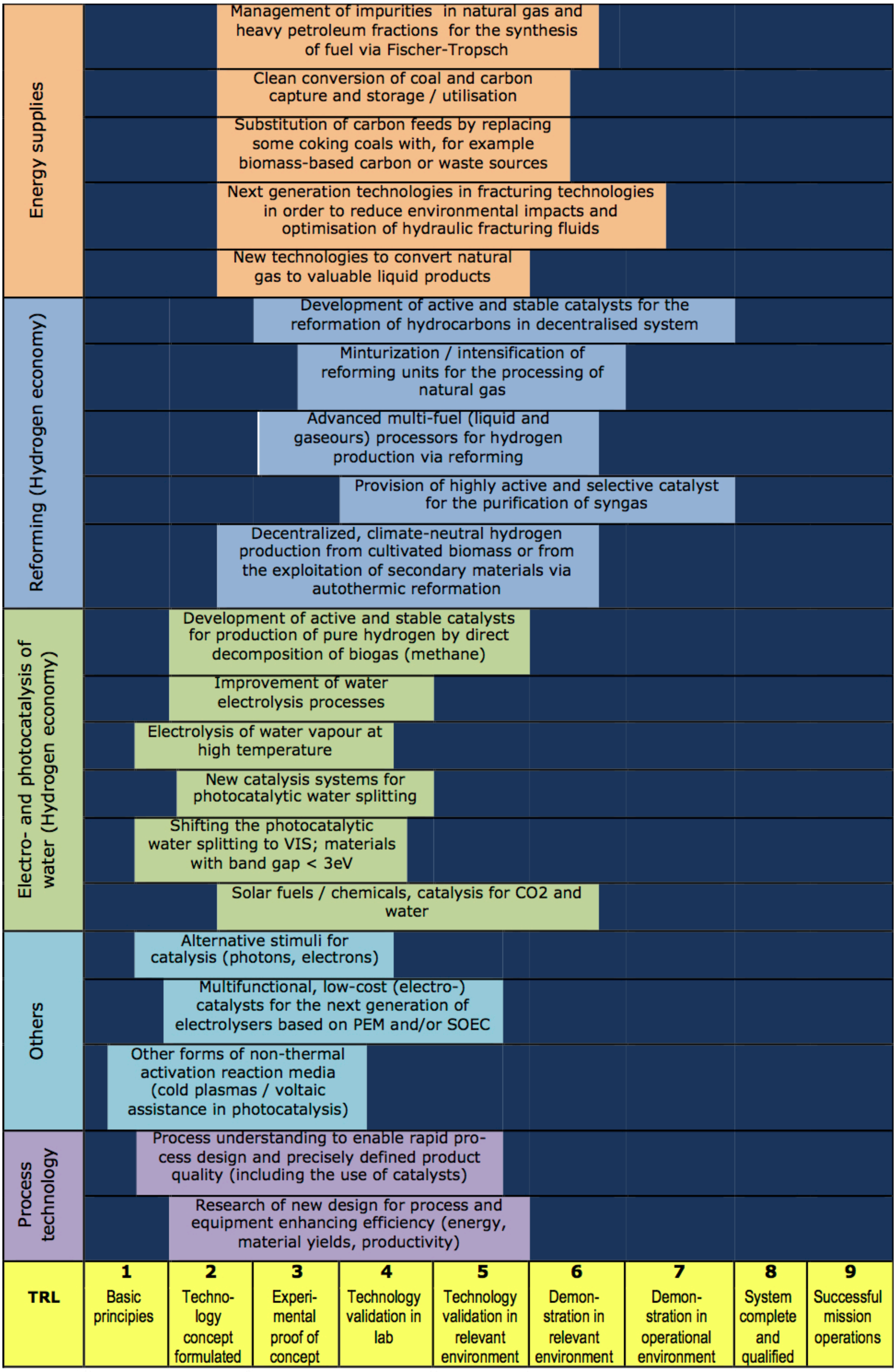
The Greek catalysis roadmap highlights the following R&D areas in the two main fields of activity "Hydrogen production and storage" and "fuel cell technology":

- Development of novel, efficient and cost-effective functional materials (catalysts and catalyst supports) for new, efficient and low cost advanced multi-fuel (liquid and gaseous) processors for hydrogen production via reforming. Effort should take advantage of recent advances in (i) nano-scale synthesis and architectures, (ii) analytical tools and screening methods, and (iii) modeling/simulation of complex chemical systems including catalyst/chemical interfaces. Research should also include the design of innovative concepts for the fuel reformer, the water gas shift and the hydrogen purification steps as well as their integrated engineering.
- Development of novel multifunctional, low-cost (electro)-catalysts (and the associated manufacturing processes) for their integration in efficient and durable components and sub-systems for the next generation of electrolysers based on both Proton Exchange Membranes (PEM) and Solid Oxide Electrolysis Cells (SOEC) as well as photo-electrolyzers.
- Concerning Solid oxide Fuel Cells, the efforts should be put on (i) development of new multifunctional nano-structured (electro)-catalysts with higher activity, durability and lifetime, preferable without platinum group metals also for operation at elevated temperatures, (ii) investigation and modelling of degradation and poisoning mechanisms for identifying deterioration mechanisms and reducing contaminant effect, including catalyst support facility, (iii) development of methods for accelerated lifetime catalyst testing and (iv) development of reliable catalysts lifetime prediction methods.

In the key action "enhancing the availability and quantity of existing resources" of the SPIRE roadmap, some research activities are recommended, which have also impact on the priorities on "competitive low carbon economy" detailed below (section 5.4.1). Especially, attention is put on: (i) new technologies to convert natural gas to valuable liquid products, (ii) clean conversion of coal and carbon capture and storage/utilisation, (iii) next generation technologies in fracturing technologies in order to reduce environmental impacts and optimisation of hydraulic fracturing fluids and (iv) substitution of carbon feeds by replacing some coking coals with, for example biomass-based carbon or waste sources

Figure 2 summarizes these energy and energy efficiency priorities. Instead of a classical roadmap diagram having an axis with time to market (short, medium and long-term), the technology readiness of the topics was chosen for the abscise scale. The topics are clustered in headings, and their horizontal position in the diagram shows their level of technology readiness (TRL).

Figure 2: Priorities for a clean and efficient energy and related Technology Readiness Levels



5.3 Smart, green and integrated transport

Although the greening of transport (including electro mobility) has been advancing in the last years, it can be expected that the bulk of fuels will still be based on hydrocarbons. On the one hand, 73% of all oil consumed in Europe is used in transport, on the other hand a doubling of passenger cars within the next 20 years are roughly estimated. Therefore there is a strong need for sustainable biofuels, which will reduce the dependency on fossil fuels. This need is part of the fourth societal challenges related to transportation identified in H2020 and it also concerns the Bio-economy aspects included in the second challenge on food, agriculture and marine topics.

First-generation biofuels research, already widely developed, will be limited to novel approaches with the development of new catalysts for the production of high quality transportation fuels from either vegetable oils or fats.

Main emphasis will be given on the *second-generation biofuels*, which include a range of alternatives such as lignocellulosic ethanol, syngas based fuels, pyrolysis-oil based biofuels and others. Activities will cover the development of new catalytic conversion processes, with a view to improve cost-competitiveness of biofuels while minimising the environmental impact of biofuel production. Results are expected to expand the biomass feedstock available for biofuel production, assisting the take-off of a large biofuel industry while helping to avoid food/fuel competition for the land use. The expected impact also relates to substantial cost reduction for the production of these second-generation biofuels, while improving the energy balance and environmental impact of biofuel production.

Third-generation biofuels based on algae is also of interest to the catalysis community. The activities in this area mostly focus on the extraction of the lipids, and their valorisation to biofuels (jet and diesel) either via transesterification or hydrogenation route.

It can be added that in this very active area of biofuels and biorefineries high Technology Readiness levels are being reached, as attested by the numerous joint actions that are developed. These actions are less and less based on mainly public-public collaborations, such as in the ERA-IB ERA-Net "Towards an ERA in Industrial Biotechnology"[24] funded under FP6, but they involve more and more industrial partners as in the "European Biofuels Technology Platform"[25] or in the recently launched public private partnerships (PPP) "Bio-based Industries Consortium".[26] In this area, the Star Colibri clustering[27] elaborated within FP7 has published two documents in 2011, a "European Biorefinery Joint Strategic Research Strategic roadmap: Targets for 2020"[28] and a "Joint European Biorefinery vision for 2030".[29]

The use of natural gas for *SYNGAS production* (synthetic gas, see also section 5.2) leads to the potential production of alternative fuels such as gasoline, aviation fuels, diesel, and alcohols. The major routes, in particular the thermo-catalytic gasification and pyrolysis of bio-oils like petroleum distillates (via hydrotreatment HDT, hydrodeoxigenation HDO, catalytic cracking FCC), also open new perspectives. This demands the development of catalysts capable to withstand the harsh conditions of these processes having mixtures of varying compositions and very often highly toxic to the active phase of the conventional metal or acid/base catalyst like zeolites.

Besides the growing demand of fuels for the transport, the *treatment of the emissions* produced by the vehicles still needs to be taken into account. Commonly, the vehicles are equipped with catalytic converters, which convert toxic by-products of combustion in the exhaust of the engine to less toxic substances. These oxidation and/or reduction reactions are best catalysed with metals form the platinum group of metals, but these are very expensive. Therefore it is of strategic importance to reduce the precious metal content of the catalysts and to develop alternative

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[24] http://www.era-ib.net/
[25] http://www.biofuelstp.eu/
[26] http://biconsortium.eu/
[27] http://www.star-colibri.eu/
[28] http://beaconwales.org/uploads/resources/Vision_2020_-_European_Biorefinery_Joint_Strategic_Research_Roadmap.pdf
[29] http://www.star-colibri.eu/files/files/vision-web.pdf

catalysts materials for catalytic converters. This field can be widened for the treatment of industrial emissions, with particular focus on:

- Development of long-term stable NO_x storage catalytic converters which are already effective at low temperatures (in order to improve NO_x storage) but can also be operated continuously at higher temperatures for improved removal of sulphur.
- Increased temperature stability of catalyst carriers.
- Decrease the light-off temperature of oxidation catalysts.
- Catalyzed particulate filters which are so active during normal operation that soot is continuously burned off the filter.

In recent years, the European automotive industry has managed to significantly reduce both fuel consumption and emissions. This was achieved by the development of gasoline engines operating with a lean air/fuel ratio with direct gasoline injection, the optimization of diesel engines, the reduction of the sulphur content of fuels and the development of highly efficient exhaust gas purification system. For both gasoline and diesel engines, the key to further reductions is to further optimize the lean operating modes. The associated increase in NO_x emissions and the necessarily lower exhaust gas temperatures will need to be overcome with more efficient catalysts. In order to comply with the Euro VI limits it is thought that a system will need to comprise at least the following four components: DOC (Diesel oxidation catalysts), CSF (Catalysed soot filter), SCR (selective catalytic reduction) and AMOX (ammonia oxidation catalyst).

The Greek, Spanish and German catalysis roadmaps outline very precisely the field of activities in biofuels (with especially topics on "Catalytic production of biofuels of new-generation" and "Decomposition and depolymerisation of cellulose and lignine") as well as in fuels for the future. The detailed targets are as follows:

Enzymatic/catalytic pre-treatment and hydrolysis of lignocellulosic biomass for ethanol production

- Research should focus on optimising the enzymatic degradation of lignin for efficient separation of cellulose and hemicellulose for subsequent enzymatic hydrolysis.
- Development of new and improved enzymes (e.g. thermostable enzymes) and supported enzyme systems, with a view to improving the rate of enzymatic hydrolysis and enzyme recycling in the whole lignocellulose to ethanol process.
- Development of combined enzymatic and oxidation/cracking activity of supported enzymes and oxidation catalysts for the simultaneous improved hydrolysis of cellulose and/or hemicellulose and degradation of lignin in the whole lignocellulose to ethanol process.

Thermochemical conversion of biomass

- Develop new catalytic systems for catalytic biomass pyrolysis towards production of bio-oil with improved physical and chemical properties.
- Explore the stability of new catalytic systems due to metal deposition originated from biomass.
- Develop new catalytic systems for the upgrading of biomass pyrolysis liquors towards high quality gaseous or liquid fuels.
- Develop catalysts and reactors for upgrading biomass pyrolysis vapors via C-C coupling reactions such as ketonization and aldol condensation.
- Development of mesoporous zeolites for hydroisomerization and hydrocracking of biomass-derived fuels components for producing high quality transportation and aviation fuels.
- Explore the development of catalysts aimed at biomass gasification including gas cleaning and conditioning techniques for further syngas utilization.
- Development of new F-T catalysts towards production of synthetic fuels through a BtL process.
- Development of new catalytic system for upgrading of F-T products produced in a BtL process.
- Hydroisomerization of long chain paraffins, wax catalytic cracking and hydrocracking are between the processes to be investigated.

- Development of new catalytic material for the selective conversion of syn-gas to ethanol and higher alcohols. Emphasis will be given to stable catalyst very selective to alcohol production.

Fuels of the future

- Design of novel reactors for decentralized low capacity synthesis gas production and Gas to Liquid (GTL) products,
- Production of synthesis gas from renewable resources with subsequent GTL ("gas to liquids") processes,
- Development of new catalysts: (i) with high activity and syngas selectivity, (ii) for direct conversion of methane into higher hydrocarbons and (iii) for conversion of synthesis gas to ethanol and higher alcohols.
- Development of solar energy based fuels with emphasis in the discovery and design of sustainable energy efficient systems.
- Development of reactor systems for the concurrent processing of fossil with biomass based components.
- Upgrading of heavy crudes to transportation fuels with emphasis in environmentally friendly marine fuels.

Moreover, as outlined in the German and Dutch catalysis roadmaps, research aiming the reduction of precious metal content should not be limited to the post-treatment of exhaust gases from internal combustion engines. Improved understanding of metal sintering behaviours, as well as development of precious metal-free catalysts and/or of catalysts that require only a very low precious metal content on account of the use of suitable carriers and additives, are needed. Reduction of precious metal will also be reached by replacing them by less expensive (e.g. transition) ones, such as Fe, Mn or Ni.

5.4 Environment, Resource efficiency and Raw materials

The H2020 societal challenge "Climate change, environment, resource efficiency and raw materials" identified by the commission is strongly concerned by catalysis and process technology improvements, with some important aspects that are analysed successively in separate sections.

5.4.1 Competitive low carbon economy

Low-carbon energy can be achieved through processes or technologies that generate substantially lower amounts of carbon dioxide emissions than presently emitted from conventional fossil fuel power plants. Low carbon power generation sources such as biomass utilisation, fuel cells and photocatalysis lead to a hydrogen economy as outlined in section 5.1. Important targets are *CO_2 valorisation*, *carbon-capture technologies for storage and recycling* (CCS and CCR) purposes and *reduction of CO_2 emissions* by improving chemical processes through catalysis.

In order to mitigate the CO_2 footprint in energy intensive industry, the *recycling of CO_2* while simultaneous producing valuable products is an economic and environmental friendly option. CO_2 can be a source of carbon for the production of hydrocarbons, monomers for polymers (e.g. polycarbonates), synthetic fuels (alcohols, hydrocarbon), fertilizers and food. CO_2 as C1-building block faces some disadvantages due to its thermodynamic stability (CO_2 is the product of combustion) and its kinetic inertness. Therefore, conversion processes need a lot of energy, preferably coming from renewable sources of H_2, or they follow a photochemical, thermochemical, electrochemical or biochemical pathway supported by catalysts. The development of appropriate catalysts for each kind of reactions proposed is a fundamental issue. A range of conversion pathways exists including production of chemicals like urea, methanol, cyclic carbonates and salicyclic acid. The emerging strategies embrace CO_2 based polymers, dry reforming, hydrogenation to formic acid, the conversion of CO_2 to acetic, acrylic or benzoic acid or further more smart materials like Polyurethane (PUR) or organic carbonates.

Another very attractive way is the *electrocatalytic* and in particular *photocatalytic reduction of CO_2*, modelled on natural process of photosynthesis. However, further developments in the heterogeneous and homogeneous catalysts systems known today are needed to reach a technological level to be commercially exploited.

In order to exploit the paradigm shift of "CO_2 – from waste to value", the EU Commission held a workshop in 2011.[30] The workshop participants identified the following areas for potential future research activities:

- Production of chemicals from CO_2 (realised as a call topic in NMP within FP7).
- Advanced catalysts for CO_2 recycle technologies: Research in the field requires to develop photocatalysts for splitting water as well as novel catalysts for direct methanol synthesis from CO_2.
- Production of liquid fuels from CO_2/H_20 using solar energy (C-based energy vectors).

The research priorities of the Netherlands, Greece, Germany, Spain and France are going in the same direction:

- CO_2 usage through photocatalytic and electrocatalytic processes – modelled on natural processes (GR, DE).
- Synthesis of chemical products with high added value, in which CO_2 remains in the product as a C1 building block (NL, GR, DE, ES, FR).
- Hydrogenation of CO2 with hydrogen from renewable resources (DE, ES).
- Carbon dioxide utilization for the production of fuels / solar fuels - including catalysis for CO_2 and water (NL, GR, FR).

At above cited EU-workshop, it was agreed by the experts that “CO_2 sequestration and capture technologies that allow separation of CO_2 from process streams with further storage or recycling are now commercially available”, based on the efforts performed within FP7 on some topics focussed on CCS technologies. Nevertheless, still a particular need for research is felt by Greece in technology development for the capture and utilization of carbon dioxide during the production and use of fossil fuels. Besides, since several call topics dedicated to the use of CO_2 have been already published within the NMP Work Programme of FP7, one of them dealing specifically with “Fine chemicals from CO_2” (see table 2), the follow-up call topics should be rather centred on enhanced research and innovation in this field.

The SPIRE Roadmap already presented in section 4.1 is also concerned with optimal valorisation of exhaust gases emitted at various stages in the process industries, and is therefore engaged in developments towards a low carbon economy. In *conversion of CO_2 to value-added products*, CO_2-derived polymers and fine chemicals are approaching the stage of commercial introduction. As the next challenge, SPIRE identifies the multi-electron reduction of CO_2 to fuels. Besides, the CO_2 reduction should involve investigations in the feed section in industrial production processes, aiming greater energy and resource efficiency. This can be reached through optimal valorisation and smarter use of existing, alternative and renewable feedstock, as well as by improved production processes including energy technologies and management concepts, efficient systems and equipment or materials. For instance, novel efficient heat and energy storage technologies will be significant for the industries in order to balance their energy consumption by means of fully integrated and monitored processes: this includes storage of energy at different temperatures, development of processes at different temperatures compared to today’s technology and development of cooling, solidification or cleaning processes with heat recovery instead of water quenching. Similarly, reduction of the CO_2 emissions by industries should be reached by applying more sustainable processes (development of novel materials with less CO_2 and energy footprint down the value chain, e.g. LEDs, PVs, etc.) and by creating new sustainable materials that will help the process industry itself to develop more energy and resource efficient processes (i.e. energy storage materials, materials for high temperature processes).

In the recently published "Technology Roadmap – Energy and GHG Reductions in the Chemical Industry via Catalytic Processes", developed by IEA (International Energy Agency), ICCA (International Council of Chemical Associations) and DECHEMA (Society for Chemical Engineering

[30] http://ec.europa.eu/research/industrial_technologies/pdf/co2-workshop-30032011_en.pdf

and Biotechnology),[31] an important key finding was that catalyst and related process improvements could reduce energy intensity for the manufacture of 18 major products by 20% to 40% as a whole by 2050, leading to savings of 1 gigaton (GT) of CO_2 equivalent per year by 2050 versus a "business-as-usual" scenario. Its research recommendations, outlined in the annex 9 of this roadmap,[32] are also relevant to the other headings of the present document, like energy, mobility and biomass. Concerning the utilisation of CO_2, the following research areas are promoted:

- Photocatalytic or electrocatalytic activation modelled on natural processes.
- Synthesis of products with high added value, in which CO_2 remains in the product as a C1 building block (for example polycarbonates, polyurethane).
- Hydrogenation of CO_2, with hydrogen from regenerative sources.

Other research recommendations in this document concern *improved feedstock efficiency* and *new routes to polymers* using new catalytic technologies for the production of olefins and aromatic compounds (or their direct secondary products) from natural gas. Also, more energy-efficient methods for monomer production and polymerisation are considered, enabled by catalytic and process engineering R&D. It is stressed that for transformation of short-chain alkanes from natural gas, in particular for the C1 building block methane, carbon-linking reactions activation as well as reaction focussed on the introduction of double bonds will play a decisive role. The following points are amongst the priorities in this area:

- Dehydrogenation of propane to propylene
- Partial oxidation of alkanes with oxygen for direct production of methanol, ethanol, acetic acid, propanol and acrylic acid
- New techniques and catalysts for the production of monomer building blocks on the basis of new raw materials
- Improvement of the mechanical stability of powdery and formed catalyst types
- Optimisation of resistance to catalyst poisons
- Better control of product distribution for more efficient and sustainable use and recycling of raw materials

Above aspects are also widely supported by the German and Greek national roadmaps that have also expressed some additional specific research priorities:

- Activation of C1-C4 alkanes for the production of high added value chemicals and oxygenates through nanostructured catalyst development
- Development of new energy efficient selective catalytic processes for the valorisation of C1-C4 alkanes

5.4.2 Water innovation: boosting its value for Europe

The access to clean drinking water is a human right, acknowledged at the General Assembly of the United Nation on 28 July 2010. In addition, maintaining an adequate, quality water supply is essential for agricultural productivity. Recent studies show that competing demands for scarce water resources may lead to an estimated 40% global water supply shortage by 2030, also effecting large parts of Europe.[33] Innovative technologies for *water and wastewater treatment* are needed: Energy efficient desalination processes as well as novel membranes, catalytic and photochemical processes for the removal of a range of contaminants from waste water. Efficient catalytic water purification techniques will have a dual role in treating water, by both making it potable and also by removing contaminants from wastewater and industrial waste streams.

In the FP7 programme, in NMP, several topics were dedicated to water treatment, focused on development of *(nano-)membranes*. One topic concerning on photocatalytic materials for depollution is funding a project developing a novel generation of low-cost nano-engineered photocatalysts for sunlight-driven water depollution. Indeed, *heterogeneous photocatalysis* is a

[31] see Table 3
[32] http://www.dechema.de/dechema_media/Downloads/Positionspapiere/IndustrialCatalysis/Chemical_Roadmap_2013_Annexes.pdf
[33] http://www.mckinsey.com/client_service/sustainability/latest_thinking/charting_our_water_future

robust technology for water (and air) treatment. In heterogeneous photocatalysis two or more phases are used in the reaction as well as light-absorbing semiconductors in order to initiate the photoreaction. The catalysts can carry out substrate oxidations and reductions simultaneously. Preferably, solar light should be used. The catalyst itself is unchanged during the process and no consumable chemicals are required. Additionally, because the contaminant is attracted strongly to the surface of the catalyst, the process will continue to work at very low concentrations allowing sub part-per-million consents to be achieved. Altogether, photocatalysis is a promising method for an energy and cost efficient water treatment.

On industrial sites, water is used for fabricating, processing, washing, diluting, cooling or transporting a product. In the past two decades, the closure of water loops in several industries, like in the pulp and paper industries, was a prominent task, enabled by developments in membrane technologies. Process steps need to be improved or adapted. Water, but also the diluted components could be recycled. Industrial developments still require further improvements, technologies or a new approach. For example, the production of chemicals from biomass by means of industrial biotechnology will often lead to a situation that the product has to be separated from a relatively dilute and complex aqueous stream. Closure of the water, nutrients and minerals cycles in these novel industrial processes will require novel developments in water technologies

Amongst others, the German Catalysis Roadmap and the Spanish, French and Italian priorities in catalytic water and waste water purification are: (i) development of new catalysts for advanced oxidation of organic contaminants, (ii) increasing the selectivity and long-term stability of catalysts in order to reduce inorganic contaminants in groundwater and wastewater and (iii) development of catalysts for in situ applications in contaminated groundwater aquifers – nanocatalysis. In addition, the SPIRE roadmap proposes recommendations focused on the process and process control, especially on (i) systems and tools (including in-line monitoring) for assessment and control of quantity and quality of process water and (ii) control of impurities in closed water cycles including monitoring tools and highly selective separation processes.

5.4.3 Raw materials and wastes

As already outlined in section 5.3, *replacing rare earth and precious metals* represents a challenging target for catalysis. Precious metals like platinum are of strategic relevance for the chemical industry and especially for catalysis. One prominent example deals with the catalytic exhaust-gas converter: each catalyst contains about 3g of precious metals, mostly platinum and palladium, applied on ceramic carriers. Precious metals are important for large chemical processes for producing bulk chemicals as well as in the hydrogenation and dehydrogenation processes in refineries. In accordance with the raw materials initiative of the EU[34] and regarding the cost efficiency, the availability and the dependence on imports, it is highly recommended to reduce and in the best case to replace the precious metal content in catalysts. This position is supported by all CAPITA's partners countries, and is especially highlighted by the Netherlands, Germany, Greece, France and Spain. The objective to be reached is either (i) the replacement of toxic/noble/scarce metals in catalysts by non-toxic/non-noble/abundant metals or (ii) the complete or partial removal of rare earth and precious metals through optimisation of catalysts

The efficient *use of biomass, residues and waste streams as chemical feedstock* is another important target that requires substantial R&D effort in catalysis. In order to convert lignocellulosic feedstock into biobased chemicals and materials, the main tasks for catalysis are the depolymerisation and selective decomposition of functional groups of cellulose, hemicellulose, carbohydrates and other biogenic compounds, as well as their re-functionalization. This requires that the catalysts are stable in water, since most of the biomass-based processes are operating in aqueous systems. Biocatalysts (bacteria, enzymes or yeasts) which allow for a significant increase of conversion rate and yield and are operating under mild condition should be taken into account. Here a direct link to the biobased economy is given and is reflected in a wider scope in the

[34] http://ec.europa.eu/enterprise/policies/raw-materials/critical/index_en.htm

strategic papers of the PPP BioBased Industries Consortium as well as in the European Industrial Initiative on bioenergy of the SET-Plan.[35]

In the national catalysis roadmaps of the Netherlands, Spain and Germany, several topics are dedicated to biomass conversion to chemicals and material (for details on biofuels see section 5.3). These topics are supported in the Technology Roadmap of the IEA:[36]

- Biomass conversion to chemicals (NL)
- Decomposition and depolymerisation of cellulose and lignine (DE, ES)
- New catalysts for conversion of biomass-derived feedstocks (ES)
- Development of emulsion-stable catalysts /carrier materials (DE, ES)

The Greek catalysis roadmap emphasises the aqueous processing with following research recommendations:

- Development of water stable catalysts for conversion of bio feedstocks components to chemicals or biofuels.
- Development of new catalytic materials for biomass matrix opening and hydrolysis of cellulose and hemicellulose components.
- Development of catalysts with high selectivity towards the production of platform chemicals (furanics, Lellulinic acid, et al) via hydrolysis of xylose or pentose components

The French perspective on the valorisation of biomass as chemical feedstock lies on the process technology. Several steps are required: extraction, separation and synthesis of the biomolecules. Developments are linked to the related field of polymers, where new catalysts are needed to improve the properties of the products (particularly an improved tacticity control).

In the SPIRE Roadmap, two additional topics related to biomass processing technologies are also present: (i) new pre-treatment processes to facilitate further selective fractionations and processes and (ii) new selective biotechnical, chemical, thermal, and catalytic processes for the conversion of the biomass fractions to the desired raw materials that can be converted into speciality and bulk products, including platform chemicals.

5.5 Development in catalysts and reactor concepts

The combination of a reaction stage with selective material separation in a device could reduce the number of process steps and thus lead to process intensification. New membrane materials developments stimulate further R&D in this field. For example, catalytic porous membranes are one approach to largely *eliminate materials transport inhibitions* between reaction phases and within porous catalysts. Here, the porous structure of the membrane and the arrangement of the catalyst within the contact zone play a key role. The German Catalysis Roadmap identified some research targets in the field of multifunctional reactors that consist in (i) elaborating new, cost-effective preparation techniques for multi-functional catalytic active membranes and (ii) developing catalytic systems with long-term stability which are permanently coupled to membranes.

In *micro-structured reactors* where the dimensions of the flow channels in the reactors are downsized, it is possible to run catalysed reactions at the kinetic limit, i.e. the reactor (material and heat transport) does not limit the catalyst output. The advantages of the performance of chemical processes in these microstructures are that the lateral temperature and concentration gradients are reduced and in the case of heavily endo- and exothermal reactions can be better controlled. France and Germany strongly suggest the exploitation of the potential of microreactor and micro-structured reactor technologies in catalysis. This includes the development of new high-performance catalysts, new process windows and new synthesis/reaction routes, as well as the establishment of methods and correlations for the design of catalysed processes in microstructured reactors both in terms of reaction technology and technical safety.

[35] http://setis.ec.europa.eu/implementation/technology-roadmap/european-industrial-initiative-on-bioenergy
[36] see Table 4

Hybrid catalysis can also combine solutions from different catalysis fields, focused on the integration of functionalities – e.g. enzyme catalysis, bio-mimicking catalysts, homogeneous and heterogeneous catalysts – in order to simplify the production process of chemicals from commodity chemicals to pharmaceuticals. Hybrid catalysis is particularly suitable for multicomponent systems, complex substrates and cascade reactions. This would in principle include a nanotechnology approach to catalysis, integrating nanoparticles with enzymes etc. The Dutch catalysis roadmap identifies following topics on (i) fully exploitation of the developments in hybrid catalysis, (ii) development of a new toolbox of methods and (iii) identification of the right hybrid interface ("niche").

For the optimisation of catalysts and of catalytic processes, the understanding of the performance of the catalyst under the specific conditions of the reaction is also highly valuable. With the recent progresses in characterisation techniques and calculations methods, a dual approach gives now the possibility, on one hand, to observe a catalyst as accurate as possible when operating (i.e. *in situ investigations* of catalysts using *operando methods*) and, on the other hand, to model an active surface without oversimplification by using quantum chemical methods like density functional theory (DFT) or kinetic Monte Carlo (MC) simulation. Combined with the statistical correlations derived from high-throughput experimentations, these breakthroughs could pave the way for validated and really predictive quantitative structure–activity relationship (QSAR) models. In this domain, there are several research recommendations in the German Catalysis Roadmap, supported by the French roadmap:

- Development of operando methods of catalyst characterisation for high-throughput experimentation.
- Development of analytical operando techniques for solid catalysts under process-relevant conditions (pressure, temperature, flow reactors, coupling with online product analysis), with coupling of several operando methods for simultaneous investigation of a sample under identical conditions.
- Adaption of in situ methods for online monitoring of catalyst synthesis.
- Theoretical understanding of catalytic processes through quantum chemical treatment and simulation of sufficiently large model systems with the necessary precision.
- Coupling of quantum chemical methods with approaches from the field of molecular mechanics (QM / MM coupling) in order to calculate complex systems like the active centre of enzymes or the modelling of active surfaces.

In addition, the Dutch catalysis roadmap identified following research topics in the exploitation of non-linear dynamics in catalysis: (i) catalyst as a dynamic system, understanding and exploiting the "life" of a catalyst, (ii) exploit dynamics: non-stationary transient catalysis, non-stationary operation, nonlinearities, oscillations, (iii) self-repairing catalysts and (iv) smart dynamic polymers for catalysis.

6. Conclusions

The ERA-Net CAPITA, initiated within FP7, was launched in 2012 when the transition of the European Framework Programme towards H2020 was going on. The CAPITA roadmap beneficiates from all the reflexions made during this period and, as a result, the priorities meet numerous topics of the Societal Challenges identified as important for the future of Europe by the Commission. All partners' countries also contributed through the identification of national priorities in the domain. A further advantage of this roadmap is that it gathers a significant number of recent documents and roadmaps focussed on area in which Catalysis and Process Technology play a major role, namely energy, environment or bio-economy, amongst others. From all these national and international contributions, the preservation of the very large place of catalysis in the world to come and its ability to evolve to answer energy and environmental requirements are highlighted.